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We analyse the ground state of a particle in a double-well potential, with a cylindrical symmetry, and in the presence of a magnetic field. We find that the azimuthal quantum number m takes the values $m = 0, 1, 2, \dots$ when we increase the magnetic field. At critical values of the magnetic field, the ground state is twice degenerate. The magnetisation shows an oscillatory behaviour and jumps at critical values of the magnetic field. This phase transition could be seen in the condensate of a dilute gas of charged bosons confined by a double-well potential.

I. INTRODUCTION

It is a well-known fact¹ that in the absence of a magnetic field the ground state of bosons is non degenerate, and therefore has the symmetry of the hamiltonian. Mathematically this result from the fact that the kernel of the operator e^{-tH} is positive. This last property no more holds in the presence of a magnetic field so that degeneracy of the ground state may be expected, as well as symmetry breaking in it. One-body systems already may show this phenomenon. Indeed Lavine and O'Carroll² proved the existence of spherically symmetric potentials for which, in the presence of a magnetic field, the ground state has a non-vanishing value for the z component of angular momentum, so that the rotational symmetry is broken.

Further examples were provided by Avron, Herbst and Simon^{3,4}. On the opposite side, these last authors were able to prove that for the hydrogen atom the symmetry is not broken, as well as in the case where the potential is monotonically increasing with the distance. These authors, however, mainly concerned with problems of atomic physics, did not discuss the degeneracy and the physical significance of it.

On the other hand, two of us analysing the problem of a particle confined to a disc or an annulus in the presence of a magnetic field found that the ground state was degenerate in the case of an annulus and for a disc with Neumann boundary conditions (with Dirichlet boundary conditions in the disc case the degeneracy disappears.) The degeneracy appears each time the magnetic field reaches a critical value and the magnetisation jumps at these critical values, which form a discrete set⁵.

Motivated by these results we consider in this article a class of systems for which similar phenomena occur. Namely we analyse the ground state of a particle in three dimensions moving in a double-well type potential, cylindrically symmetric, and submitted to a constant magnetic field in the z direction.

We find that the ground state has an azimuthal momentum $\hbar m$ taking increasing values $m = 0, 1, 2, \dots$ when we increase the magnetic field B . At critical values of B (B_m) the ground state is twice degenerate between the m and the $m + 1$ state. Moreover the magnetisation jumps at these critical values and shows in general an oscillatory behaviour reminiscent of the well known de Haas von Halphen oscillations in solid state physics.

We show that this phenomenon can be understood by an analysis of the minima of the potential energy, fixing however the angular momentum to its quantised value $\hbar m$. In the two-dimensional case we can use the WKB method and obtain bounds on the energy in order to estimate the critical fields. But in general, we had to compute numerically the energies and compare them to estimates based on trial wave functions. The agreement is quite good in general.

Concerning possible experimental verifications of these effects, which require basically to have a potential which has a minimum sufficiently far from the origin, we could think of two cases. The first one would be in some molecules where proton dynamics could be described by such an effective potential. The second one, more thrilling, would be the case of charged bosons undertaking a Bose-Einstein condensation. Our results suggest that in this case, the bosons would undertake a **phase transition** in their condensate, when we apply an increasing magnetic field. This phase transition would manifest itself by appearance of oscillations in the **magnetisation**, which would **jump** at certain critical values of the magnetic field.

II. THE MODEL

We will consider the case of a particle of mass μ , charge q , in a potential V with a cylindrical symmetry, submitted to a magnetic field \vec{B} in the z direction. We do not consider the effect of the spin of the particle. We choose

for a unit of energy V_0 , and length r_0 , both being characteristic of the potential. The dimensionless hamiltonian reads if $r = \sqrt{x^2 + y^2}$

$$(i\epsilon \vec{\nabla} - \vec{A})^2 + V(r, z) \quad (1)$$

where

$$\epsilon = \frac{\hbar}{r_0 \sqrt{2\mu V_0}} \quad (2)$$

measures the importance of the quantum effects and the vector potential in the symmetric gauge is given by

$$\vec{A} = \left(\frac{-By}{2}, \frac{Bx}{2}, 0 \right) \quad (3)$$

$B = \frac{q}{c} \frac{r_0}{\sqrt{2\mu V_0}} \tilde{B}$ being the dimensionless magnetic field.

Thanks to the cylindrical symmetry, we can replace the z component of the angular momentum L_z by its eigenvalue ϵm so that the reduced hamiltonian reads

$$H_m = -\epsilon^2 \left[\frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} \right] + \left(\frac{\epsilon m}{r} - \frac{rB}{2} \right)^2 + V(r, z) \quad (4)$$

The ground state energy of this hamiltonian and the corresponding eigenfunction will be denoted E_m and ψ_m .

It remains to specify V . We will basically consider a double-well potential of the form:

$$V(r, z) = r^4 + z^4 - 2(r^2 + z^2) + v r^2 z^2 \quad (5)$$

with v satisfying $v \geq -2$, so that V is bounded from below. If v is equal to 0 we can decouple the motion in the z direction from the one in the plane perpendicular to the magnetic field. This is what we will call the **two-dimensional case**. If $v = 2$, we have in three dimensions a potential with spherical symmetry.

We have chosen this double-well form because if we had taken the simple well $V = r^4 + z^4 + 2(r^2 + z^2) + v r^2 z^2$ with $v \geq 0$ it follows from³ that the ground state is not degenerate and corresponds to $m = 0$.

A physical quantity of interest is the **magnetisation** in the ground state

$$M = -\frac{\partial E}{\partial B} \quad (6)$$

in units $\frac{q}{c} r_0 \sqrt{\frac{V_0}{2\mu}}$

We will denote by e_m the ground state energy of the hamiltonian

$$h_m = -\epsilon^2 \left[\frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} \right] + V_m(r, z) \quad (7)$$

with

$$V_m = \frac{(\epsilon m)^2}{r^2} + \frac{B^2}{4} r^2 + V \quad (8)$$

and by

$$E_m = e_m - \epsilon m B \quad (9)$$

the ground state energy of H_m given in (4), so that the real ground state energy is given by

$$E = \inf_{m \geq 0} E_m \quad (10)$$

since obviously negative m give a larger energy.

Finally we will use the following useful scaling property of the energy e_m

$$e_m(\epsilon, \lambda, v) = s^2 e_m\left(\frac{\epsilon}{s^{3/2}}, \frac{\lambda}{s}, v\right) \quad \forall s \geq 0 \quad (11)$$

where

$$\lambda = \frac{B^2}{4} - 2 \quad (12)$$

is the parameter multiplying r^2 in the potential. Equation (11) follows simply from the scaling transformation : $r^2 \rightarrow s r^2$ and $z^2 \rightarrow s z^2$. This relation shows that we have effectively a two parameter dependence of the energy e_m in general and a one parameter dependence in the two dimensional case.

The choice $s = |\lambda|$ or $s = m^{\frac{1}{3}}$ ($m \geq 1$) shows that large magnetic field or large angular momenta correspond to the semi-classical limit. In fact we shall see that in the classical limit $\epsilon \rightarrow 0$ ground state with $m \neq 0$ are favoured inducing ground state degeneracies at some values of the magnetic field. It thus appears that the tendency to have a ground state with the same symmetry as the hamiltonian and therefore non degenerate is an effect due to quantum mechanics.

III. THE CLASSICAL LIMIT

One can gain some qualitative understanding of the problem by looking at the classical limit of it. This means that we neglect the quantum kinetic energy and define the ground state energy as

$$E = \inf_{m \geq 0} \inf_{(r, z)} [V_m(r, z) - \epsilon m B] \quad (13)$$

where

$$V_m = \frac{(\epsilon m)^2}{r^2} + r^4 + z^4 + \frac{B^2}{4} r^2 - 2r^2 + v r^2 z^2 \quad (14)$$

and consider that m is an integer.

Two cases need to be considered separately: $|v| < 2$ and $v \geq 2$. If $|v| < 2$ we denote by x_m and t_m respectively the values of r^2 and z^2 which minimise the potential V_m , and we find

$$t_m = 1 - \frac{v x_m}{2} \quad (15)$$

$$\left(2 - \frac{v^2}{2}\right) x_m + \left(v - 2 + \frac{B^2}{4}\right) = \frac{(\epsilon m)^2}{x_m^2}$$

On the other hand, considering for a while m as a continuous variable, the absolute minimum of $V_m - \epsilon m B$ is given by

$$\epsilon \hat{m} = \frac{B}{2} x_{\hat{m}} \quad (16)$$

From (15) this gives an absolute minimum of $V_m - \epsilon m B$ given by

$$x_{\hat{m}} = t_{\hat{m}} = \frac{1}{1 + \frac{v}{2}} \quad (17)$$

and therefore

$$\epsilon \hat{m} = \frac{B}{2} \frac{1}{1 + \frac{v}{2}} \quad (18)$$

In considering the variable m as a continuous one we have treated the problem purely classically and the corresponding "ground state" energy is

$$E^{cl} = -\frac{2}{1 + \frac{v}{2}} \quad (19)$$

We know that m is a discrete variable but for consistency we must consider ϵ as a small number. Then if m designates the integer part of \hat{m} , we have $\hat{m} = m + \theta$ and if $0 \leq \theta < \frac{1}{2}$, the ground state has the quantum number m , whereas if $\frac{1}{2} < \theta \leq 1$ it has $m + 1$.

From this analysis we conclude that if $B_{m-1} < B < B_m$ where

$$B_m = \epsilon(1 + \frac{v}{2})(2m + 1) \quad (20)$$

the ground state has the quantum number m . Hence we see that by increasing the magnetic field, we find in increasing order the values of $m = 0, 1, 2, \dots$ and an infinite set of **critical values of the magnetic field exist**, B_m for which the ground state is twice **degenerate**, being both m and $m + 1$.

This picture is entirely confirmed by the numerical results in the quantum case. It is also quite interesting to look at the magnetisation. In the state whose quantum number is m , we have

$$M_m = \epsilon m - \frac{B}{2} x_m \quad (21)$$

so that using (15)

$$M_m = [\epsilon m - \frac{B}{2} \frac{1}{1 + \frac{v}{2}}] [\frac{1 - \frac{v}{2}}{1 - \frac{v}{2} + \frac{B^2}{4}}] \quad (22)$$

when $B_{m-1} < B < B_m$.

This shows that the magnetisation has an "oscillatory" type of behaviour reminiscent of the familiar de Haas von Halphen one in solid state physics and that the **magnetisation jumps at the critical values of the magnetic field**, the jump being given by

$$\Delta M_m = \epsilon \frac{1 - \frac{v}{2}}{1 - \frac{v}{2} + \frac{B^2}{4}} \quad (23)$$

Once again this general behaviour is reproduced by the numerical results in the quantum case and the spacing between the values of the critical field is rather well represented by formula (20) when $m \geq 1$. In the **two-dimensional** case, i.e. $v = 0$ and neglecting the trivial z dependence, we can proceed further and look at a really semi-classical approximation namely WKB, for the ground state energy

$$\int_{r_-}^{r_+} dr \sqrt{e_m - V_m(r)} = \frac{\epsilon \pi}{2} \quad (24)$$

where

$$V_m(r) = \frac{(\epsilon m)^2}{r^2} + r^4 + (-2 + \frac{B^2}{4})r^2 \quad (25)$$

and the ground state energy is $E_m = e_m - \epsilon m B$.

In fact this WKB approximation will give the best analytical results, apart from the variational estimates for the energy, which give unfortunately only exact upper bounds on the energy.

When the potential has spherical symmetry $v = 2$, quantum effects are much more important and the classical analysis gives only that the ground state has $m = 0$ if $B < 2\epsilon$, is degenerate between $m = 0$ and $m = 1$ when $2\epsilon \leq B < 4\epsilon$, has possibly $m = 0, 1, 2$ for $4\epsilon \leq B < 6\epsilon$ and so on. This only suggests that we have again the increasing sequence of m , when we increase the magnetic field and that critical values appear near $2\epsilon m$.

When $v > 2$, we find that $m = 0$ is the ground state except when $B = 2\epsilon m$, where it is degenerate between m and 0. We may note however that the classical ground state correspond to points $(r = 0, z = \pm 1)$ in configuration space for $m = 0$, whereas it corresponds to two circles $(r = \frac{\epsilon}{2B}, z = \pm \sqrt{1 - \frac{\epsilon}{2B}})$ for $m = 1$ and $2\epsilon < B < 4\epsilon$, so that the wave function can be more spread in the $m = 1$ state than in the $m = 0$ state, and that the kinetic energy of the $m = 1$ state is lower, favouring the $m = 1$ state. Hence we should expect, at least when ϵ is small, a ground state with $m = 0$ for small fields and a ground state with $m = 1$, when $2\epsilon < B < 4\epsilon$. A similar argument can be given for the higher values of m .

Finally, it is worth noticing that if we had taken a simple well type potential

$$V(r, z) = r^4 + z^4 + 2(r^2 + z^2) + v r^2 z^2 \quad (26)$$

the classical analysis gives a ground state with $m = 0$, at least when $v \geq -1$. This is a correct result when $v \geq 0$ at the quantum level.

IV. NUMERICAL RESULTS AND VARIATIONAL BOUNDS

It is quite useful to undertake a numerical analysis of this problem. We have used a finite element method, choosing for the basis a product of two triangles functions. We discuss separately the two-dimensional problem and the three dimensional ones.

A. Two dimensions

We first give pictures of the ground state energy for two typical values of ϵ , a small ($\epsilon = 0.03$) and a large one ($\epsilon = 0.5$) as a function of the magnetic field B . (figure 1). The cusps at the critical values of B indicate a jump of the corresponding magnetisation.

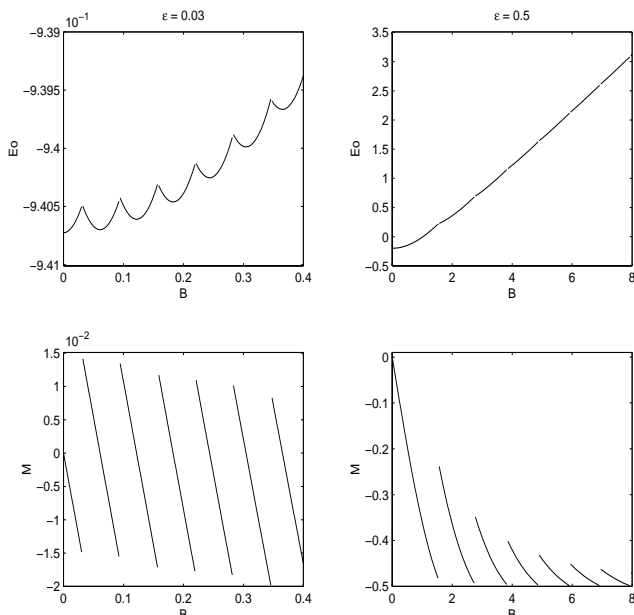


FIG. 1. Energie and magnetisation dependence of B for $\epsilon = 0.03$ and $\epsilon = 0.5$

This last quantity shows first a diamagnetic behaviour at small field, but then a paramagnetic - diamagnetic oscillation at least when $\epsilon \lesssim 0.3$. Beyond this value the magnetisation is entirely negative (figure 1 bottom right). We can also note that when B becomes large the magnetisation tends to $-\epsilon$, its value in the Landau regime.

The results clearly indicate that we go progressively from the states with $m = 0, 1, 2 \dots$ by increasing the magnetic field and that the magnetisation jumps at the critical values. The effect is more pronounced in the classical regime. All these results are in qualitative argument with the classical picture presented before and the agreement is even quantitative when $\epsilon = 0.03$ for example.

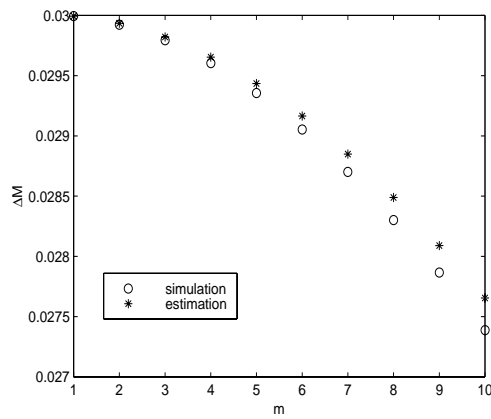


FIG. 2. Comparison of the jumps given by simulation and the estimation

The jumps of the magnetisation given by formula (22) are reproduced (figure 2) with a precision of less than 1 percent when $\epsilon = 0.03$, and the spacing between the critical values of the magnetic field

$$\frac{B_{m+1} - B_m}{\epsilon} = 2 + \Delta_m \quad (27)$$

is given by $\Delta_m \leq 0.04$ if $m \geq 1$ and $\epsilon = 0.1$. Δ_m decreases when m increases in agreement with the scaling relation $B_m = (2m + 1)\epsilon$, so that the simple classical formula reproduces rather well the results. By contrast, the jump between the $m = 0$ and the $m = 1$ state is largely of quantum mechanical origin, as well as the precise values of the critical fields.

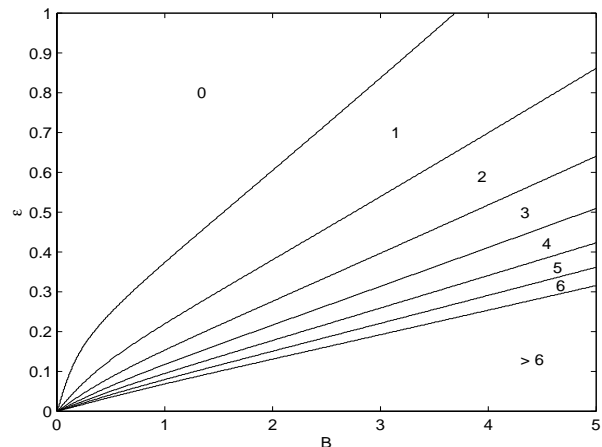


FIG. 3. M values of the ground state depending on B and ϵ

Figure 3 describes the various regions in the $\epsilon - B$ plan. We can note that even when $\epsilon > 0.25$ a linear relation exists between B_m and ϵ , as in the classical regime, which is a bit surprising.

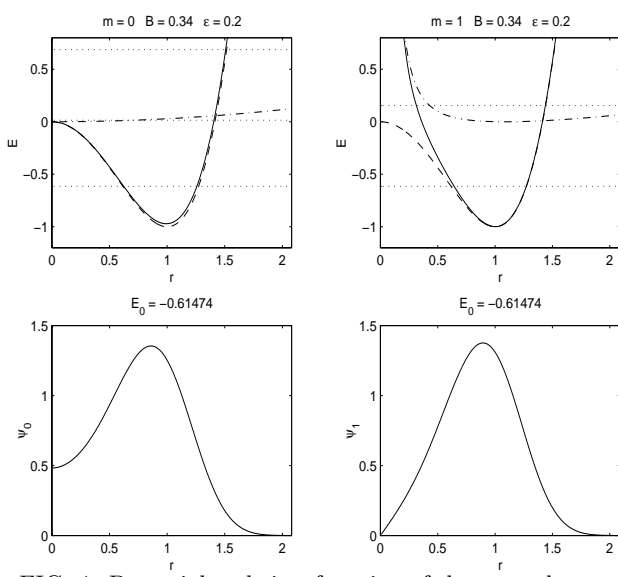


FIG. 4. Potential and eigenfunction of the ground state for $m = 0$ (left) and $m = 1$ (right) with V_m (—) = orbital kinetic energy (— · —) + double-well (— —) and energy levels (· · ·)

It is also interesting to look at the eigenfunctions when the magnetic field reaches its critical value. In figure 4 we give pictures of them at the critical value between the state $m = 0$ and $m = 1$ when $\epsilon = 0.2$. We see that their maxima are located very near the minimum of the potential.

Finally we compare the results with two theoretical estimates: first of all the WKB one, and a variational one. This last estimate is based on the following two parameters trial wave function

$$\psi_m = r^m e^{-\alpha r^2 - \beta(r-1)^2} \quad (28)$$

The variational upper bound on the energy can be expressed in terms of Weber cylindrical functions, but we directly computed the corresponding integrals.

Deg.	Simul.	WKB	$\delta \%$	Variat.	$\delta \%$
0-1	0.0313	0.0314	0.23	0.0317	1.16
1-2	0.0944	0.0942	-0.15	0.0946	0.23
2-3	0.1573	0.1571	-0.13	0.1574	0.09
3-4	0.2201	0.2198	-0.13	0.2203	0.06
4-5	0.2830	0.2826	-0.12	0.2830	0.02
5-6	0.3457	0.3453	-0.12	0.3458	0.02
6-7	0.4085	0.4080	-0.12	0.4085	0.00

TABLE I. Magnetic field B_m at the seven first degeneracies with $\epsilon = 0.03$

Deg.	Simul.	WKB	$\delta \%$	Variat.	$\delta \%$
0-1	-0.9405	-0.9401	0.66	-0.9403	0.26
1-2	-0.9404	-0.9400	0.65	-0.9403	0.27
2-3	-0.9403	-0.9399	0.64	-0.9401	0.28
3-4	-0.9401	-0.9397	0.63	-0.9399	0.29
4-5	-0.9399	-0.9395	0.61	-0.9397	0.30
5-6	-0.9396	-0.9392	0.59	-0.9394	0.30
6-7	-0.9392	-0.9389	0.56	-0.9390	0.30

TABLE II. Energies E_m at the seven first degeneracies with $\epsilon = 0.03$

Tables I,II,III and IV give a comparison of the results for two values of the parameter ϵ , and for the critical fields. Excellent agreement is found for the variational method (maximal error of the order of 2 % when $\epsilon = 0.5$). WKB works quite well when ϵ is small ($\epsilon = 0.03$) as expected, but even better on the energies when $\epsilon = 0.5$ and the error does not exceed 1%.

Deg.	Simul.	WKB	$\delta \%$	Variat.	$\delta \%$
0-1	1.538	1.661	7.95	1.508	-1.98
1-2	2.747	2.811	2.33	2.743	-0.15
2-3	3.842	3.882	1.06	3.842	0.02
3-4	4.891	4.919	0.56	4.894	0.05
4-5	5.920	5.940	0.34	5.924	0.07
5-6	6.941	6.954	0.18	6.943	0.02
6-7	7.953	7.964	0.12	7.956	0.02

TABLE III. Magnetic field B_m at the seven first degeneracies with $\epsilon = 0.5$

Deg.	Simul.	WKB	$\delta \%$	Variat.	$\delta \%$
0-1	0.220	0.232	0.97	0.227	0.55
1-2	0.685	0.686	0.04	0.690	0.25
2-3	1.159	1.159	-0.02	1.163	0.16
3-4	1.639	1.638	-0.03	1.642	0.12
4-5	2.122	2.122	0.00	2.125	0.12
5-6	2.609	2.608	-0.02	2.612	0.07
6-7	3.098	3.098	0.00	3.101	0.07

TABLE IV. Energies E_m at the seven first degeneracies with $\epsilon = 0.5$

B. Three dimensions

For the spherically symmetric potential ($v = 2$), figure 5 gives the ground energies as well as the corresponding magnetisation for two different values of ϵ : 0.03, 0.5.

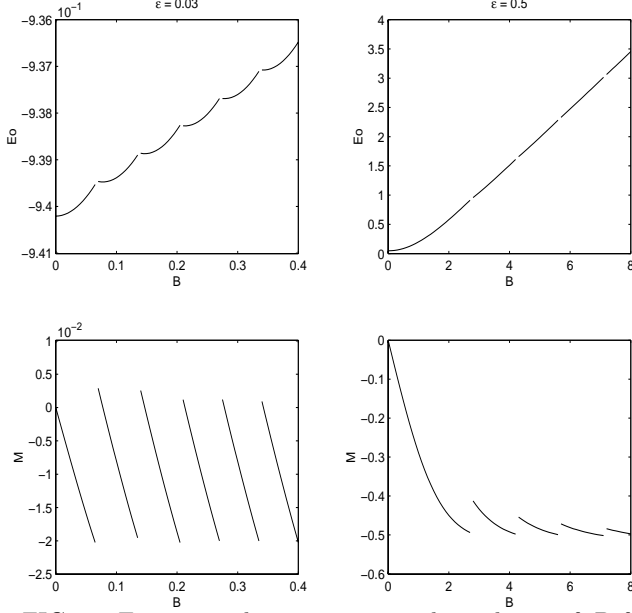


FIG. 5. Energie and magnetisation dependence of B for $\epsilon = 0.03$ and $\epsilon = 0.5$

Once again we see that the values of m in the ground state increases with B , and that the magnetisation jumps at critical values B_m of the magnetic field, where the ground state is doubly degenerate. These results are in qualitative agreement with the classical analysis. Figure 6 summaries the results in the $\epsilon - B$ plane. Notice that in this

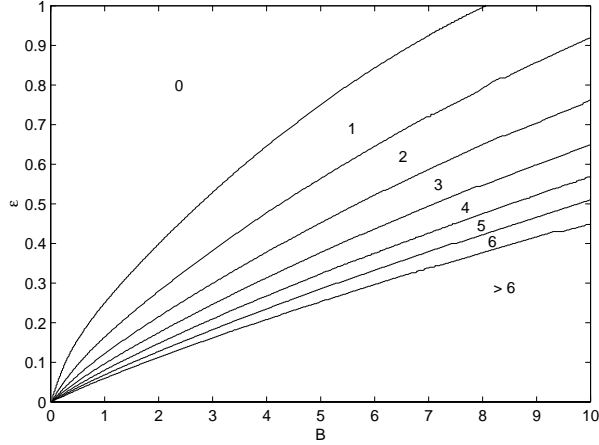


FIG. 6. M values of the ground state depending on B and ϵ

case, when $\epsilon \geq 0.1$ already the relation between B_m and ϵ is no more linear. On the other hand the spacing

between the critical values of B predicted by the crude classical estimate:

$$\Delta B_m = B_{m+1} - B_m \cong 2\epsilon \quad (29)$$

is satisfied with a precision of 25% at $m = 1$ and becomes more accurate when m increases, at least in the range $\epsilon \leq 0.1$.

Our best variational estimate for the energy was made with a three parameter trial wave function

$$\psi_{\alpha,\beta,\zeta} = r^m e^{-\alpha r^2 - \beta(\sqrt{r^2 + z^2} - \zeta)^2} \quad (30)$$

Table V gives the values of the critical field B_m and Table VI the corresponding ground state energies, when $\epsilon = 0.05$ estimated by the variational method and computed with the simulation.

Deg.	Simulation		Variational			
	B_m	E_m	B_m	δ_B %	E_m	δ_E %
0-1	0.1180	0.1206	2.17	-0.8986	-0.8982	0.38
1-2	0.2381	0.2310	-2.94	-0.8966	-0.8966	-0.01
2-3	0.3549	0.3509	-1.15	-0.8946	-0.8946	-0.06
3-4	0.4686	0.4616	-1.49	-0.8925	-0.8925	-0.00
4-5	0.5829	0.5785	-0.74	-0.8901	-0.8901	-0.01
5-6	0.6961	0.6905	-0.80	-0.8876	-0.8876	-0.00

TABLE V. Magnetic field B_m and energies E_m at the six first degeneracies at $\epsilon = 0.05$

Deg.	Simulation		Variational			
	B_m	E_m	B_m	δ_B %	E_m	δ_E %
0-1	2.7576	0.9415	2.6225	-4.89	0.8959	-2.34
1-2	4.2493	1.6345	4.0912	-3.72	1.5675	-2.54
2-3	5.6746	2.3190	5.4972	-3.12	2.2363	-2.49
3-4	7.0961	3.0126	7.0275	-0.96	2.9845	-0.69
4-5	8.5025	3.7055	8.2415	-3.07	3.5720	-2.83
5-6	9.7537	4.3248	9.6016	-1.55	4.2412	-1.57

TABLE VI. Magnetic field B_m and energies E_m at the six first degeneracies at $\epsilon = 0.5$

Obviously there is a very good agreement, since the largest error for B_m is less than 2% and for E_m less than 0.7%. Table VI gives the same but for $\epsilon = 0.5$. Again we see a good agreement (error less than 5%). When ϵ increases we found that α increases and β decreases as well as ζ and our trial wave function becomes less accurate, because the double-well nature of the potential is less important compared to the kinetic energy.

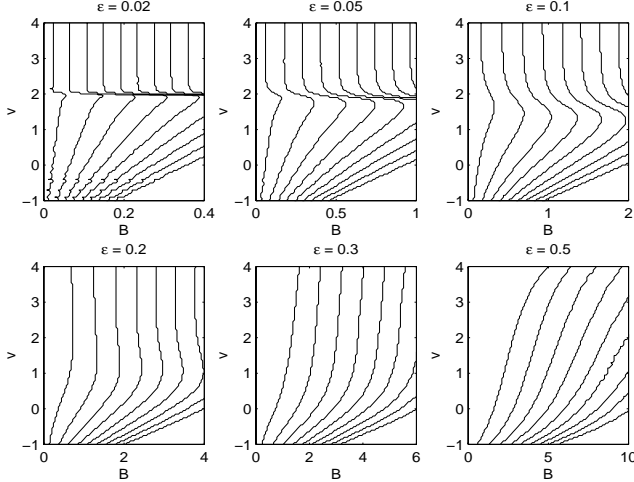


FIG. 7. M values of the ground state depending on B and v with increasing ϵ

Figure 7 describes the situation in the $v - B$ plane for $m = 0, 1, \dots, 10$ and different values of ϵ . We notice that when v is less than 2 and ϵ is not too large ($\epsilon \leq 0.2$), the situation is similar to the one already discussed, but that there is an abrupt change at $v = 2$ when ϵ is small in agreement with the classical analysis. However when $\epsilon > 0.2$ the ground state $m = 0$ is definitely favoured as v increases.

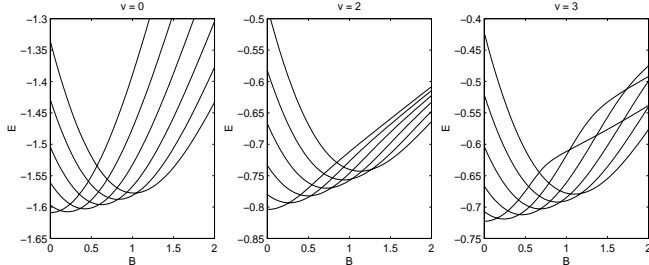


FIG. 8. Comparison for different v of the energy for $m = 0, 1, 2, 3, 4, 5$ depending on B with $\epsilon = 0.1$

Figure 8 shows the energies for the first five m values computed with three different v : two-dimensional ($v = 0$), spherical potential ($v = 2$), and $v = 3$. We can see a new crossing between the $m = 0$ and the other m levels when v becomes larger than 2, although this does not concern the ground state.

V. BOUNDS ON THE CRITICAL FIELD IN THE TWO DIMENSIONAL CASE

One might desire to get rigorous upper and lower bounds on the critical fields. One possible approach would consist in getting upper and lower bounds on the ground state energies E_m . Whereas we have seen that one can obtain very good variational upper bounds, it is rather difficult to get good lower ones. In order to test these results, we analysed only the two-dimensional case.

First we want to obtain conditions under which $m = 0$ is the ground state. Using the inequality

$$\frac{l^2}{x} + x^2 \geq x^2 - \frac{l^2}{a^2}x + \frac{2l^2}{a} \quad (31)$$

valid for any x and a positive, we deduce that

$$e_0[\lambda] \geq \frac{2(\epsilon m)^2}{a} + e_0\left[\lambda - \left(\frac{\epsilon m}{a}\right)^2\right] \quad (32)$$

On the other hand

$$\begin{aligned} e_0[\lambda] - e_0\left[\lambda - \left(\frac{\epsilon m}{a}\right)^2\right] &= \int_{\lambda - (\frac{\epsilon m}{a})^2}^{\lambda} d\lambda' \langle r^2 \rangle_0(\lambda') \\ &\leq \left(\frac{\epsilon m}{a}\right)^2 \langle r^2 \rangle_0\left[\lambda - \left(\frac{\epsilon m}{a}\right)^2\right] \end{aligned} \quad (33)$$

since $\langle r^2 \rangle_0(\lambda)$ is decreasing in λ .

But

$$|\langle r^2 \rangle_0[\lambda] - \frac{\lambda}{2}| \leq \left[e_0[\lambda] + \left(\frac{\lambda}{2}\right)^2\right]^{\frac{1}{2}} \quad (34)$$

The scaling relation and the fact that e_0 is increasing in ϵ imply that when $\frac{\lambda}{2} \leq -1$

$$e_0[\lambda] + \left(\frac{\lambda}{2}\right)^2 \leq \left(\frac{\lambda}{2}\right)^2 (e_0[-2] + 1) \quad (35)$$

Taking now a such that $\frac{\epsilon m}{a} \geq \frac{B}{2}$ ($m \geq 1$) we get combining these inequalities that

$$E_0 \leq E_m \quad \forall m \geq 1 \quad (36)$$

if we can find $t > \frac{B}{2}$ such that

$$t^2 \left\{ 1 + \frac{1}{2} \left(t^2 - \frac{B^2}{4} \right) \right\} \delta - 2\epsilon \left(t - \frac{B}{2} \right) < 0 \quad (37)$$

where $\delta = 1 + \sqrt{e_0[-2] + 1}$

In the estimate for δ we can use our best variational upper bound. Inequality (37) will be satisfied if B is less than some value B_0 , so that in this range $m = 0$ is the ground state. In order to see when $m \neq 0$ is a ground state, we use the following trial wave function $\psi(r)$ for a state with angular momentum m' .

$$\psi(r) = r^{m'-m} \psi_m(r) \quad m' \geq m \quad (38)$$

where $\psi_m(r)$ is the exact ground state wave function for the state with angular momentum m . An integration by parts shows that

$$\begin{aligned} \int_0^\infty dr r [\psi_m'^2 r^{2(m'-m)} + 2(m'-m)r^{2(m'-m)-1} \psi_m' \psi_m] \\ = - \int_0^\infty dr r^{2(m'-m)} \psi_m (r\psi_m)' \end{aligned} \quad (39)$$

Therefore if we use the fact that

$$\frac{\epsilon^2}{r} (r\psi_m')' = [V_m(r) - e_m] \psi_m \quad (40)$$

We see that

$$\begin{aligned} \int_0^\infty dr r [\epsilon^2 \psi'^2 + V_{m'}(r) \psi^2] = e_m \int_0^\infty dr r \psi^2 \\ + \epsilon^2 2m'(m'-m) \int_0^\infty dr r^{2(m'-m)-1} \psi_m^2 \end{aligned} \quad (41)$$

and we conclude that

$$e_{m'} \leq e_m + \epsilon^2 2m'(m'-m) \frac{\langle r^{2(m'-m-1)} \rangle_m}{\langle r^{2(m'-m)} \rangle_m} \quad (42)$$

In particular

$$e_1 \leq e_0 + 2\epsilon^2 \frac{1}{\langle r^2 \rangle_0} \quad (43)$$

If we have a lower bound c on $\langle r^2 \rangle_0$ then we see that

$$E_1 < E_0 \quad (44)$$

if

$$B > \frac{2\epsilon}{c} \quad (45)$$

We can use for the lower bound c the one given in equation (34)

$$c = \frac{\lambda}{2} - \sqrt{e_0[\lambda] + \left(\frac{\lambda}{2}\right)^2} \quad (46)$$

which is satisfactory when B is not too large, but which becomes negative for large B . We can repair this by using the fact³ that if f is an increasing function of r , its expectation value in the ground state is lowered by adding to the potential a new increasing potential. We can find a useful comparison potential

$$W = a_1 r^2 + a_2 r^4 + a_3 r^6 \geq V \quad (47)$$

which has a ground state wave function of the form

$$\psi = e^{b_1 r^2 - b_2 r^4} \quad b_2 > 0 \quad (48)$$

so that $\langle r^2 \rangle_W$ can be computed explicitly for this potential and we can take $c = \langle r^2 \rangle_W$ in equation (45), which gives a more satisfactory result for large B .

In any case we see that the state $m = 1$ is favoured over the state $m = 0$ if B is larger than some value, and by continuity there must exist a field for which both states have equal energy. But in order to prove that the ground state is $m = 1$ when B is in some range requires to show that $E_m > E_1 \forall m \geq 2$. For this purpose let us consider m as a continuous parameter. Then

$$\frac{\partial E_m}{\partial m} = 2\epsilon^2 m \langle \frac{1}{r^2} \rangle_m - \epsilon B \quad (49)$$

If we can show that $\frac{\partial E_m}{\partial m} \geq 0$ for all $m \geq 1$, then we will have shown that $E_m > E_1$. When $m \geq 1$ we have

$$\langle \frac{1}{r^2} \rangle_m \geq \frac{1}{\langle r^2 \rangle_m} \quad (50)$$

and

$$\frac{(\epsilon m)^2}{\langle r^2 \rangle_m} + \langle r^2 \rangle_m^2 + \lambda \langle r^2 \rangle_m \leq e_m \quad (51)$$

In order to get a variational bound on e_m we can use the trial wave function $\psi = r^m e^{-ar^2}$, which gives

$$e_m \leq \frac{m+1}{m+2} V_{m+2}(x_{m+2}) \quad (52)$$

where x_m is the value of x which minimises

$$V_m(x) = \frac{(\epsilon m)^2}{x} + x^2 + \lambda x \quad (53)$$

Noting that equation (51) implies that

$$\langle r^2 \rangle_m \leq x_m + \sqrt{e_m + V_m(x_m)} \quad (54)$$

one can see by combining equations (49), (50), (52) and (54) that $E_m > E_1$ for all $m \geq 2$ if

$$\frac{B^2}{8} < \frac{1}{1+c^2} \quad (55)$$

with

$$c^2 = \frac{1}{\epsilon^2} |\lambda| \left[x_1 + \sqrt{V_{1+2m}(x_{1+2m}) - V_1(x_1)} \right]^2 \quad (56)$$

which implies that B should be less than some value.

We give in the table VII some numerical values for the bounds obtained by these methods.

ϵ	$E_0 < E_1$	B_{0-1}	$E_1 < E_m$	B_{1-2}	$E_1 < E_0$
0.01	0.0 - 0.005	0.011	0.0 - 0.026	0.030	0.022 -
0.05	0.0 - 0.024	0.054	0.0 - 0.124	0.163	0.146 -
0.1	0.0 - 0.047	0.121	0.0 - 0.221	0.359	0.366 -
0.2	0.0 - 0.088	0.340	0.0 - 0.364	0.878	1.788 -
0.5	0.0 - 0.189	1.610	0.0 - 0.609	2.745	2.834 -
1.0	0.0 - 0.310	3.686	0.0 - 0.826	5.846	4.277 -
2.0	0.0 - 0.469	7.816	0.0 - 1.066	11.910	8.141 -

TABLE VII. Results of the inequalities on the energies and values B_m

They show that whereas the range of values of B for which $E_0 < E_1$ and $E_1 < E_0$ is reasonably estimated for $\epsilon \lesssim 0.1$, there is no range of values of B for which our bounds show that $m = 1$ is the ground state except when ϵ is very small (0.01). But in this range WKB works perfectly well. Obviously we have too poorly estimated the effect of the kinetic energy and that of the centrifugal barrier. Numerical computations for example show that the replacement of $\langle \frac{1}{r^2} \rangle_1$ by $\frac{1}{\langle r^2 \rangle_1}$ is not appropriate when ϵ or B are too large.

In conclusion, even in two dimensions improved rigorous bounds on the critical values of the magnetic field are needed, and the WKB method for which we have no estimate of the error gives the best analytic results.

VI. CONCLUSION

It could be of course quite interesting to see an experimental verification of these surprising effects of the magnetic field. Even though we have found them in the case of a double-well, we think that the details of the potential do not matter too much. What is needed is a potential whose minimum is taken sufficiently far from the origin.

We have thought of two possible fields where one could observe such effects. The first one is molecular physics where often the dynamics of electrons or protons is modelled by the motion of a quantum particle in a double-well (although admittedly often a one-dimensional one.) If we consider the case of the electron in the rotationally symmetric double-well, the smallest value of the critical field where the $m = 1$ and $m = 0$ states are degenerate is about 15 Tesla if we take for the depth of the potential 1 eV and for the distance to the origin of the minimum 2 Å. For protons the situation is more favourable since a field of 5 Tesla can create a degeneracy when the depth is kept to 1 eV and the minimum is at a distance of 1.5 Å. Obviously a more detailed investigation is needed if one wants to see these unusual effects (like a change from diamagnetism to paramagnetism) in molecules.

The other field is that of Bose-Einstein condensates of very cold atoms, which recently has made spectacular progress. If we consider free charged bosons in a magnetic field and in a potential $V(\frac{r}{r_0})$ one can show that there is a Bose-Einstein condensation in the ground state in three dimensions, in the limit r_0 going to infinity, for all potentials which have a quadratic dependence of r near the origin. Our result supports therefore that free charged bosons in their condensate would show a phase transition when one varies the magnetic field. This transition would manifest itself by jumps of the magnetisation at some critical values of the magnetic field. The phenomenon would probably persist in a dilute gas of charged bosons in a neutralising background. It is however probably quite difficult to create such a jellium in the laboratory and this remains a challenging task.

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